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Molecular Dynamics Simulation of High Strain-Rate Void Nucleation and Growth in Copper[1] J. BELAK, D.B. BOERCKER, G.S. BALES, J. GLOSLI, University of California, Lawrence Livermore National Laboratory, Livermore, CA 94551 — Isotropic tension is simulated in nanoscale polycrystalline copper with 10nm grain sizes using large-scale molecular dynamics. The nanocrystalline copper is fabricated on the computer by growing randomly oriented grains from random positions in the simulations cell. Constant volume strain rates of 10^8 - 10^{10} are considered for systems ranging from 10^5 - 10^6 atoms using an EAM interatomic potential for copper. The spacing between voids for room temperature simulations is found to scale approximately as $l \sim 0.005 * C_s/\dot{\epsilon}$, where C_s is the sound speed and $\dot{\epsilon}$ is the strain rate. Below strain rates of about 10^9, only one void is observed to nucleate and grow in the simulation cell. The growth of small voids is simulated by cutting a void out of the simulation cells and repeating the isotropic expansion. Results are presented for several grain boundary orientations (textures) and void sizes and compared to macroscopic models.

[1]Work performed under the auspices of the U.S. DOE by LLNL under contract No. W-7405-ENG-48.

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